Heat transport in disordered quantum harmonic oscillator chains

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We study heat conduction in quantum disordered harmonic chains connected to general heat reservoirs which are modeled as infinite collection of oscillators. Formal exact expressions for the thermal current are obtained and it is shown that, in some special cases, they reduce to Landauer-like forms. The asymptotic system size dependence of the current is analysed and is found to be similar to the classical case. It is a power law dependence and the power depends on the spectral properties of the reservoirs.

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In an earlier paper [1]we studied the problem of heat conduction in a classical disordered harmonic chain that is connected to heat baths specified by general spectral functions. In this paper we use the formalism, developed by Ford, Kac, and Mazur [2] (FKM) to model quantum mechanical heat reservoirs, and extend our earlier calculations to the quantum mechanical regime. Our results should be useful in interpreting recent experiments [3] on heat transport in insulating nanowires and nanotubes. They are also of interest in the context of the question of validity of Fourier's law in one-dimensional systems, a problem that has received much attention recently [4].

As pointed out in an earlier paper [9], on transport in Fermionic wires, the FKM method seems to be a powerful and relatively straightforward method for studying nonequilirium transport. Here we use this formalism to obtain exact results for the heat current in a disordered harmonic chain. Landauer's result, suitably generalized to the phononic case, is obtained as a special case. For general reservoirs the conductance of a wire depends on details of the reservoirs and contacts. Our analysis here closely follows the one followed in [1,5,6] for the case of classical oscillator chains. The results obtained in the classical oscillator case and the present problem have a lot of formal similarity which of course is because both the problems are linear. There has been some earlier work on quantum wires [7,8] which follow a similar approach but we give a more clear and complete picture and make some interesting predictions for experiments.

We consider a mass disordered harmonic chain containing N particles with the following Hamiltonian:

$$H=\sum_{l=1}^{N}\frac{p_l^2}{2m_l}+\sum_{l=1}^{N-1}\frac{(x_l-x_{l+1})^2}{2}+\frac{(x_1^2+x_N^2)}{2} \qquad (1)$$

where $\{x_l\}$ and $\{p_l\}$ are the displacement and momentum operators of the particles and $\{m_l\}$ are the random masses. Sites 1 and N are connected to two heat reservoirs (L and R) which we now specify. We model each reservoir by a collection of M oscillators. Thus the left reservoir has the following Hamiltonian:

$$\begin{aligned}H_L&=\sum_{l=1}^{M}\frac{P_l^2}{2}+\sum_{l,m}\frac{1}{2}K_{lm}X_lX_m \qquad (2)\\ &=\sum_{s=1}^{M}\frac{\tilde{P}_s^2}{2}+\frac{\omega_s^2}{2}\tilde{X}_s^2=\sum_{s=1}^{M}(n_s+1/2)\omega_s a_s^\dagger a_s,\end{aligned}$$

where K_{lm} is a general symmetric matrix for the spring couplings, $\{X_l,P_l\}$ are the bath operators and $\{\tilde{X}_l,\tilde{P}_l\}$ are the corresponding normal mode operators. They are related by the transformation $X_l=\sum_s U_{ls}\tilde{X}_s$ where U_{ls}, chosen to be real, satisfies the eigenvalue equation $\sum_l K_{nl}U_{ls}=\omega_s^2 U_{ns}$ for $s=1,2...M$. The annihilation and creation operators a_s, $a_s^\dagger$ are given by $a_s=(\tilde{P}_s-i\omega_s\tilde{X}_s)/(2\omega_s)^{1/2}$, etc. and $n_s=a_s^\dagger a_s$ is the number operator.

The two reservoirs are initially in thermal equilibrium at temperatures T_L and T_R. At time $t=\tau$ the system, which is in an arbitrary initial state is connected to the reservoirs. We consider the case where site 1 on the system is connected to X_p on the left reservoir while N is connected to $X_{p'}$ on the right reservoir. Thereafter the whole system evolves through the combined Hamiltonian:

$$H_T=H+H_L+H_R-kx_1X_p-k'x_NX_{p'}.$$

The Heisenberg equations of motion of the system variables are the following (for $t>\tau$):

$$\begin{aligned}m_1\ddot{x}_1&=-[2x_1-x_2]+kX_p\\ m_l\ddot{x}_l&=-(-x_{l-1}+2x_l-x_{l+1}) \quad 1<l<N\\ m_N\ddot{x}_N&=-[-x_{N-1}+2x_N]+k'X_{p'}. \qquad (3)\end{aligned}$$

We note that they involve the bath variables $X_{p,p'}$. However these can be eliminated and replaced by effective noise and dissipative terms, by using the equations of motion of the bath variables. Consider the equation of motion of the left bath variables. They have the form:

$$\begin{aligned}\ddot{X}_n&=-K_{nl}X_l \quad n\neq p\\ \ddot{X}_p&=-K_{pl}X_l+kx_1 \qquad (4)\end{aligned}$$

This is a linear inhomogeneous set of equations with the solution

$$X_n = \sum_l [F_{nl}(t-\tau)X_l(\tau) + G_{nl}(t-\tau)\dot{X}_l(\tau) + \int_\tau^\infty dt' G_{np}(t-t')kx_1(t') \quad \text{where} \tag{5}$$
$$F_{nl}(t) = \theta(t)\sum_s U_{ns}U_{ls}\cos(\omega_s t);$$
$$G_{nl}(t) = \theta(t)\sum_s U_{ns}U_{ls}\frac{\sin(\omega_s t)}{\omega_s}.$$

Thus we find that X_p (say) appearing in Eq. (3) has the form $X_p(t) = h(t) + k\int_\tau^\infty dt' G_{pp}(t-t')x_1(t')$. The first part, given by $h(t) = \sum_l [F_{pl}(t-\tau)X_l(\tau) + G_{pl}(t-\tau)\dot{X}_l(\tau)$, is like a noise term while the second part is like dissipation. The noise statistics is easily obtained using the fact that at time $t=\tau$ the bath is in thermal equilibrium and the normal modes satisfy $\langle a_s^\dagger(\tau)a_{s'}(\tau)\rangle = f(\omega_s,\beta_L)\delta_{ss'}$. Here $f = 1/(e^{\beta\omega}-1)$ is the equilibrium phonon distribution and $\langle\hat{O}\rangle = Tr[\hat{\rho}\hat{O}]$ where $\hat{\rho}$ is the reservoir density matrix and Tr is over the reservoir degrees of freedom. We define the Fourier transforms: $x_l(\omega) = \frac{1}{2\pi}\int_{-\infty}^\infty dt x_l(t)e^{i\omega t}$, $G^+_{pp}(\omega) = \int_{-\infty}^\infty dt G_{pp}(t)e^{i\omega t}$ and $h(\omega) = \frac{1}{2\pi}\int_{-\infty}^\infty dt h(t)e^{i\omega t}$. Taking limits $M\to\infty$ and $\tau\to-\infty$ we get:

$$X_p(\omega) = h(\omega) + kG^+_{pp}(\omega)x_1(\omega) \tag{6}$$
$$\langle h(\omega)h(\omega')\rangle = I(\omega)\delta(\omega+\omega') \quad \text{where}$$
$$I(\omega) = \frac{f(\omega)b(\omega)}{\pi}$$
$$G^+_{pp}(\omega) = \sum_s \frac{U_{ps}^2}{\omega_s^2-\omega^2} - ib(\omega) \quad \text{and}$$
$$b(\omega) = \sum_s \frac{\pi U_{ps}^2}{2\omega_s}[\delta(\omega-\omega_s) - \delta(\omega+\omega_s)].$$

Similarly for the right reservoir we get $X_{p'} = h'(\omega) + k'G^+_{p'p'}(\omega)x_N(\omega)$, the noise statistics of $h'(\omega)$ being now determined by β'. The left and right reservoirs are independent so that $\langle h(\omega)h'(\omega')\rangle = 0$. We can now obtain the particular solution of Eq. (3) by taking Fourier transforms and plugging in the forms of $h(\omega)$ and $h'(\omega)$. We then get:

$$x_l(t) = \int_{-\infty}^\infty \hat{Z}^{-1}_{lm}(\omega)h_m(\omega)e^{i\omega t} \tag{7}$$
$$\hat{Z} = \hat{\phi}_{lm} - \hat{A}_{lm} \quad \text{with}$$
$$\hat{\phi}_{lm} = -(\delta_{l,m+1} + \delta_{l,m-1}) + (2 - m_l\omega^2)\delta_{l,m}$$
$$\hat{A}_{lm} = \delta_{l,m}[k^2G^+_{pp}(\omega)\delta_{l,1} + k'^2G^+_{p'p'}(\omega)\delta_{l,N}]$$
$$h_l(\omega) = kh(\omega)\delta_{l,1} + k'h'(\omega)\delta_{l,N}.$$

We can now proceed to calculate steady state values of observables of interest such as the heat current and the temperature profile. We first need to find the appropriate operators corresponding to these. To find the current operator $\hat{j}$ we first define the local energy density $u_l = \frac{p_l^2}{4m_l} + \frac{p_{l+1}^2}{4m_{l+1}} + \frac{1}{2}(x_l - x_{l+1})^2$. Using the current conservation equation $\partial\hat{u}/\partial t + \partial\hat{j}/\partial x = 0$ and the equations of motion we then find that $\hat{j}_l = (\dot{x}_l x_{l-1} + x_{l-1}\dot{x}_l)/2$. The steady state current can now be computed by using the explicit solution in Eq. (7). We get

$$\langle\hat{j}_l\rangle = \int_{-\infty}^\infty d\omega(i\omega)[k^2\hat{Z}^{-1}_{l,1}(\omega)\hat{Z}^{-1}_{l-1,1}(-\omega)I(\omega) + k'^2\hat{Z}^{-1}_{l,N}(\omega)\hat{Z}^{-1}_{l-1,N}(-\omega)I'(\omega)] \tag{8}$$

The matrix Z is tridiagonal and using some of its special properties [9] we can reduce the current expression to the following simple form:

$$\langle\hat{j}_l\rangle = \frac{k^2k'^2}{\pi}\int_{-\infty}^\infty d\omega\frac{\omega b(\omega)b'(\omega)}{\mid Y_{1,N}\mid^2}(f-f') = \int_{-\infty}^\infty d\omega J(\omega)(f-f') \tag{9}$$

where $J(\omega) = k^2k'^2\omega b(\omega)b'(\omega)/\pi\mid Y_{1,N}\mid^2$ has the physical interpretation as the total heat current in the wire due to all right-moving (or left-moving) scattering states of the full Hamiltonian (system + reservoirs). Such scattering states can be obtained by evolving initial unperturbed states of the reservoirs with the full Hamiltonian [9,10]. We have denoted by $Y_{l,m}$ the determinant of the submatrix of $\hat{Z}$ beginning with the lth row and column and ending with the mth row and column. Similarly let $D_{l,m}$ denote the determinant of the submatrix formed from $\hat{\Phi}$.

For the special case when the reservoirs are also one dimensional chains with nearest neighbor spring constants $K_{lm} = 1$ and the coupling constants k, k' are set to unity, we have: $G^+_{pp} = G^+_{p'p'} = e^{-ik}$ where $\omega = 2\sin(k/2)$, $I(\omega) = f(\omega)\sin(k)/\pi$ for $\mid\omega\mid < 2$ and $I(\omega) = 0$ for $\mid\omega\mid > 2$. In this case Eq. (9) simplifies further and has an interpretation in terms of transmission coefficients of plane waves across the disordered system. We get:

$$J = \frac{1}{4\pi}\int_{-2}^2 d\omega\omega|t_N(\omega)|^2(f-f') \quad \text{where} \tag{10}$$
$$|t_N(\omega)|^2 = \frac{4\sin^2(k)}{|D_{1,N_s} - e^{ik}(D_{2,N_s} + D_{1,N_s-1}) + e^{i2k}D_{2,N_s-1}|^2}$$

is the transmission coefficient at frequency ω. We have thus obtained the Landauer formula [11] for phononic transport. It is only in this special case of a one-dimensional reservoir and perfect contacts that we get the Landauer formula. The reason is that, only in this case is the transmission through the contacts perfect, and this requirement is one of the crucial assumptions in the Landauer derivation. Note that in Eq. (10) (i)the transmission coefficient *does not* depend on bath properties and (ii) transmission is only through propagating modes. For general reservoirs where we need to use

Eq. (9) the factor $J(\omega)$ involves not just the properties of the wire but also the details of the spectral functions of the reservoirs. Thus the conductivity of a sample can show rather remarkable dependence on reservoir properties as we shall see below. The above Landauer-like-formula has earlier been stated in [12] and derived more systematically in [13]. We note that in the high temperature limit T , $T' \to \infty$ Eq. (10) reduces to the classical limit obtained exactly in [1,5,6].

Asymptotic system-size dependences : In the case of electrical conduction the conductance of a long disordered chain decays exponentially with system size as a result of localization of states. In the case of phonons the long wavelength modes are not localized and can carry current. This leads to power-law dependences of the current on system size as has been found earlier in the context of heat conduction in classical oscillator chains. A surprising result is that the conductivity of such disordered chains depend not just on the properties of the chain itself but also on those of the reservoirs to which it is connected. It can be shown [1] that the asymptotic properties of the integral in Eq. (9) depend on the low frequency ($\omega \lesssim 1/N^{1/2}$) properties of the integrand. This means that we will get the same behaviour as in the classical case. The details can be found in [1,5,6]. Here we summarize some of the main results:

(i) For the one-dimensional reservoir, which corresponds to the classical Rubin-Greer model [6], we get $J \sim \frac{1}{N^{1/2}}$.

(ii) The case of reservoirs which give delta-correlated Langevin noise correspond to the classical Lebowitz model [14,5] where one gets $J \sim \frac{1}{N^{3/2}}$.

(iii) In general one gets $J \sim \frac{1}{N^{\alpha}}$ where α depends on the low frequency behaviour of the spectral functions $G_{pp}(\omega)$ and $G_{p'p'}(\omega')$ [1].

Note that the case $\alpha < 1$ leads to infinite thermal conductivity while $\alpha > 1$ gives a vanishing conductivity. Thus, depending on the properties of the heat baths, the same wire can show either a vanishing thermal conductivity or a diverging one. The usual Fourier's law would predict $J \sim 1/N$, independent of reservoirs. Thus Fourier's law is not valid in quantum harmonic chains, even in the presence of disorder. This breakdown of Fourier's law in $1D$ systems has been noted in a number of earlier studies on classical systems [4] which have looked at the effects of scattering both due to impurities and nonlinearities.

Temperature profiles: The local temperature of a particle can be determined from its average kinetic energy , $ke_l = \langle p_l^2/(2m_l)\rangle$. We get

$$ke_l = \frac{1}{2}\int_{-\infty}^{\infty} d\omega m_l \omega^2 [k^2 \hat{Z}^{-1}_{l,1}(\omega)\hat{Z}^{-1}_{l,1}(-\omega) I(\omega) + k'^2 \hat{Z}^{-1}_{l,N}(\omega)\hat{Z}^{-1}_{l,N}(-\omega) I'(\omega)] \quad (11)$$

This is straightforward to evaluate numerically for given systems and reservoirs. Here we shall consider only the special case of heat transmission through a perfect one-dimensional harmonic chain attached to one-dimensional reservoirs. For the case of perfect contacts (*i.e* $k = k' = 1$) Eq. (11) simplifies (for large N) to

$$ke_l = \frac{1}{8\pi}\int_{-\pi}^{\pi} dk \omega_k [f(\omega_k) + f'(\omega_k)]. \quad (12)$$

For $T = T'$ one can verify that this corresponds to the equilibrium kinetic energy density on an infinite chain. On the other hand if we make the couplings weak (i.e. $k, k' << 1$) then we can verify that the kinetic energy density profile for $T = T'$ corresponds to that of a finite chain of length N in thermal equilibrium (in the quantum case the equilibrium energy density *depends* on l).

In the non equilibrium case, at high temperatures, the local temperature is given by $T_l = 2ke_l$ and from Eq. (12) we get $T_l = (T + T')/2$ which is the classical result [15]. At low temperatures and imperfect contacts $k, k' \neq 1$ we evaluate the local kinetic energy profile numerically using Eq. (11). As can be seen in Fig. 1 the temperature in the bulk still has the same constant value. At the boundaries however we see a curious feature noted earlier by [15,7]: the temperature close to the hot end is *lower* than the average temperature while that at the colder end is *higher* than the average. The temperature profiles at lower temperatures are only quantitatively different.

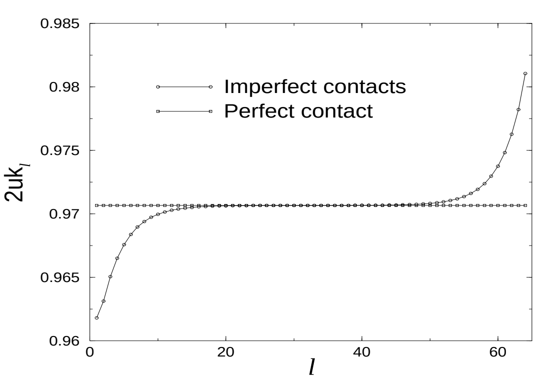

FIG. 1. Kinetic energy density profile in a pure harmonic wire (N=64) attached to one dimensional reservoirs at temperatures $T = 1$ (left) and $T' = 0.5$ (right), for perfect and imperfect contacts ($k = k' = 0.9$). The temperatures considered are quite low and so the bulk temperature is different from the classically expected value $T_{av} = 0.75$.

In summary we have used the formulation of Ford-Kac-Mazur to study heat transport in disordered quantum harmonic chains. Exact formal relations for the heat current have been derived and it is shown that one obtains Landauer-like results for special reservoirs. Earlier

results on classical chains are obtained as limiting cases. Finally we make a couple of predictions that are interesting from the experimental point of view: (i) the large system size behaviour of the heat current is a power law and the power depends on reservoir properties (ii) temperature profiles in perfect wires show somewhat counterintuitive features close to contacts. A number of experiments on heat transport in insulating nanowires have recently been carried out [3]. It would be interesting to see if our predictions, which are true for strictly one-dimensional chains, can be verified in such experiments.

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